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14. ABSTRACT
A need exists for advanced kinetics-based modeling tools to assist engine builders in the design and development of high FAR engines. Combustion Science & Engineering, Inc. (CSE) has successfully developed a flexible computational tool based on chemical reactor modeling (CRM) for the initial stages of gas turbine combustor design. Subroutines have been written in order to integrate PSR and PFR reactor codes, and to construct pathways for reactor networking. The code has been validated against experimental data for a conventional aircraft gas turbine combustor as well as a stationary gas turbine. The predictions of pollutant emissions show excellent agreement with the measurements, capturing both the magnitude and trends of the data. The input conditions to the CRM model of the aircraft combustor were extended to those of a High FAR combustor, with the expected increases in pollutant emissions and core combustion temperatures.

15. SUBJECT TERMS
Combustion, Fuel-Air Ratio, High FAR, Joint Strike Fighter, Chemical Reactor Modeling, Chemical Kinetics, Pollutant Emissions, Combustor Design

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Description of Objectives

The high fuel-air ratios and high pressure ratios required by military engine cycles present formidable challenges for combustion developers and engineers. The high overall fuel-air ratios in these cycles make achieving lean combustion (favorable for reduced NO_x emissions) in the primary combustion zone difficult. These high fuel-air ratios result in increased UHC and CO emissions and promote smoke production. The high combustor inlet pressures associated with the aggressive pressure ratios increases local flammability limits, which can result in larger smoke production regions [1]. Higher combustor inlet pressures also inhibit fuel-air mixing, which can increase NO_x emissions and further increase smoke emissions. The high combustor inlet temperatures associated with the aggressive pressure ratios also accelerate the formation of thermal NO_x. Overcoming these challenges will require creative combustion system designs to reduce emissions while meeting the demanding engine performance requirements for military engines.

Design tools are needed to facilitate the development of these new high FAR combustors. Combustor design tools can accelerate the development of new combustor technology and reduce the number of development tests required. Computational Fluid Dynamics (CFD) codes are often used in the aerothermal design process of the combustion system. Flow patterns, temperatures, and velocities are readily predicted by conventional CFD codes; however, CFD models are not readily available for estimating other quantities such as pressure losses, wall temperatures, and emissions. Other modeling tools are often employed to evaluate performance of these important combustor performance metrics. Combustion Science and Engineering, Inc. (CSE) is developing a design tool to predict pollutant formation and combustion efficiency characteristics of high FAR combustors. CSE's design tool uses chemical kinetics along with global flowfield information in functional regions of the combustor to predict NO_x, CO, and UHC emissions. This approach is often referred to as chemical reactor modeling (CRM). The CSE CRM uses a detailed chemical kinetics code to predict the emissions in key regions of the combustor. Detailed reaction chemistry is crucial for emission predictions because of the relatively slow pollution formation time scales resulting in path dependent behavior. Treatment of the detailed chemistry in a CFD code is prohibitive because of the long computational time required to evaluate the reaction chemistry at every cell in the computational domain. The CRM relies on some knowledge of the residence time and mixedness in the regions of the combustor identified to be important. CFD analysis is not needed to determine this information. These properties are determined from the combustor geometry and air distribution. This feature of the code allows for rapid estimation of the emissions performance based on the most basic of combustor design parameters resulting in an excellent preliminary design tool. The speed and simplicity of inputs to the code facilitates combustor performance evaluation over a range of operating conditions. Combustor performance maps are often prohibitive in CFD analysis because of the long times required to obtain converged solutions.

The overall objective of this program is to create an analytical tool based on chemical reactor modeling that allows the user to model aircraft gas turbine combustor as a

network of PSR's and PFR's. The model will allow a designer to conduct parametric studies in the initial stages of a gas turbine engine combustor design. The user will be able to use a graphical user interface (GUI) to choose the reactor type desired, and enter parameters as needed. The model will then solve for the rest of the unknowns to create temperature and species profiles throughout the reactor. The overall objective of Phase I was to prove the feasibility of this CRM method by creating a network of PSR-PFRs to model the gas turbine combustor. This was accomplished by identifying and evaluating appropriate detailed chemical kinetics mechanisms and by developing the computer codes necessary for exchanging data between arbitrary numbers of PSRs and PFRs. In phase I, the model was used to demonstrate its ability to predict experimental results from low FAR combustors, for which extensive experimental data was available, and showed the non-linear change in operation parameters for high FAR combustors.

Approach

The CRM uses inputs based on combustor design parameters and converts these inputs to parameters used in the detailed chemistry formulation. The input parameters related to the engine configuration and/or operating condition are:

Engine Configuration and Operation

- Combustor Air Flow Rate, W_a
- Fuel-Air Ratio, FAR
- Combustor Inlet Pressure, P_3
- Combustor Inlet Temperature, T_3

These inputs come directly from the thermodynamic cycle specified for the engine under evaluation. Inlet parameters are also required to characterize the combustor design. Air distribution and geometry inputs are defined and provided below.

Air Distribution

- Dome Flow Split
- Dome Cooling Flow Split
- Wall Cooling Flow Split
- Primary Jet Flow Split
- Dilution Jet Flow Split

Geometry

- Overall Combustor Length
- Dome Injection Location
- Primary Jet Injection Location
- Dilution Jet Injection Location

The Fuel-Air Ratio and Combustor Air Flow Rate are used to determine the Fuel Flow Rate, which is injected into the first reactor. However, all of the fuel is not consumed in

this reactor. The unreacted fuel and products are distributed into subsequent reactors based on the rules set up for the network. Rules are also established to determine what fraction of other air injection points (i.e. primary jet injection, dilution jet injection) enters the various reactors in the network. These network distribution rules are general and would be consistent over a wide range of combustor designs. It should be noted that the network inputs are directly affected by changes to the air flow distribution specified in the preliminary design phases of the combustor.

The primary jet injection location, dilution jet injection location, and overall combustor length are used to determine residence times in the reactors, respectively. The coupling of the model with the combustor geometry allows for sensitivity analysis during preliminary design stages of the combustor.

The Phase I work plan included four technical tasks. The first two tasks (Tasks 1 and 2) involved developing the computer code infrastructure for easily modeling a gas turbine combustor with an arbitrary number of chemical reactors. The next two tasks (Tasks 3 and 4) were aimed at demonstrating the ability of the CRM approach to model gas turbine combustors. Two operational gas turbine combustors, a lean, premixed power generation turbine and a conventional aircraft gas turbine combustor, were modeled to demonstrate the capability of the CRM approach (Task 3) and then the CRM tool was applied to a hypothetical high FAR combustor design in order to demonstrate the ability of the tool to accurately predict the non-linear change in combustor performance as the FAR is increased above 0.040 (Task 4).

Work Completed

Task 1 - Identify available perfectly stirred reactor (PSR) and plug flow reactor (PFR) codes, and choose an appropriate set of PSR-PFR codes.

A thorough literature and product search using engineering literature, trade publications and the World Wide Web was performed. Seven codes with the most potential were identified and checked for their ease of use, robustness, documentation, available validation data, ability to add subroutines (liquid spray model, soot production) and the ability to incorporate a detailed chemical kinetics model.

Task 2: Integrate PSR and PFR reactor codes, and construct reactor networking pathways.

The objective of Task 2 was to develop an overall program structure that allows for networking various reactor types and for the specification of flows into these reactors in order to simulate the combustor under design. A numerical code to simulate Plug Flow Reactors (PFRs), Perfectly Stirred Reactors (PSRs) and mixing regions has been developed that allows various reactor models to be combined (in any order) to simulate gas turbine combustors. This code utilizes full chemical kinetic mechanisms so that the

important phenomena that are related to the combustion chemistry, such as pollutant emissions, ignition, blowout and flameholding, can be accurately predicted.

Task 3: Demonstrate the ability of the CRM network code to predict data that exists for lean-premixed combustors.

The objective of Task 3 was to demonstrate the ability of the PSR-PFR network to predict existing pollutant data for lean-premixed combustors. Lean-premixed combustors were chosen for this validation due to the availability of experimental data, which is much more difficult to obtain for high-FAR engines. In order to complete Task 3, a thorough literature search was performed in order to obtain experimental and previous reactor simulation data. A brief list of articles is provided in the reference section. The papers cover lean premixed, aircraft engine, catalytic, and fluidized-bed coal combustors [2-6]. These papers illustrate how a variety of combustor types can be modeled by the CRM method.

A detailed study of a lean, premixed stationary gas turbine, for which detailed emissions measurements are available, was performed. A can combustor (known as Combustor A) that was studied extensively by researchers for the Department of Energy's Advanced Gas Turbine System Research Program was used as the first validation case. The results of this study are included below.

Task 4: Demonstrate the ability of the CRM network code to predict the non-linear response of combustor parameters to change in FAR, and identify parameters that have most affect on the performance of a high FAR combustor.

The goal of this task was to use the PSR-PFR network code to predict the non-linear behavior of temperature and various chemical species as a function of FARs above 0.040. If possible, the trends obtained from PSR-PFR network code would be compared to experimental data and/or analytical solutions available in literature.

This was accomplished by developing a CRM model for a conventional aircraft gas turbine combustor for which measurements of experimental pollutant emissions were available. Once the CRM model for the conventional combustor was validated, inlet conditions for a High FAR engine were used to determine the change in emissions.

Results

Overall Results

All four of the tasks outlined in the Phase I proposal have been completed successfully. The capabilities of a CRM code were demonstrated by modeling the pollutant output of two different types of gas turbines, a stationary lean, premixed combustor (Combustor A) and a conventional aircraft gas turbine combustor. The input conditions for the CRM

model of the aircraft combustor were extended to High FAR conditions to demonstrate the changes in pollutant formation under these conditions.
Accurate predictions of both NOx and CO were obtained across a range of fuel- air ratios for both the stationary gas turbine and the aircraft combustor. The model was able to provide accurate predictions of the trends of the emissions as well as the overall concentrations.

A summary of the results for the individual tasks is included below.

Task 1 - Identify available perfectly stirred reactor (PSR) and plug flow reactor (PFR) codes, and choose an appropriate set of PSR-PFR codes.

The following sets of software codes were identified as potentially viable for this product: ASPEN, CHEMCad, PRO/II, MODLINK, Cantera, CHEMKIN-II and CHEMKIN-III.

Chemical process industry flow codes (ASPEN, CHEMCad, PRO/II) can simulate various types of chemical industry processes, including PSRs and PFRs, with the ability to network the flows, however, these were excluded from further discussion because of their inability to handle large chemical kinetics reaction mechanisms. The ability to solve for detailed time-concentration histories of a large number of major and minor species including CO, NOx, and UHCs, as well as prediction of flame extinction limits, are two of the reasons why detailed chemical kinetic reaction mechanisms are important. Large mechanisms can contain well over 100 reactions, and the maximum capability of the flow codes mentioned above is well below that.

Of the other four codes identified, three codes (CHEMKIN-II, CHEMKIN-III, MODLINK) have the same origins and use the same numerical solver. CHEMKIN, a FORTRAN based suite of subroutines, originally developed by Sandia National Laboratories, is capable of solving chemically reacting flow for various types of reactors, including PSRs and PFRs. The original version of CHEMKIN (last version CHEMKIN-II) is in the public domain; however, CHEMKIN-III is currently distributed by Reaction Design, and available through license only. Reaction Design, in conjunction with Reaction Engineering, has developed a graphical user interface (GUI) version of CHEMKIN-III that allows the creation of PSR-PFR networks. This program is known as MODLINK. Figure 1 shows the interaction between subroutines and input-output files for CHEMKIN-II, CHEMKIN-III, MODLINK, and Cantera. "CORE" (in Figure 1) represents the numerical solver used by all four programs. All four codes allow large chemical kinetics reaction sets to be used, and use the same file format for accepting reaction and thermodynamic data. This allows the user to substitute one set of codes for another easily, since all that is replaced is the PSR or PFR kernel. Table 1 compares CHEMKIN-II, CHEMKIN-III, MODLINK and Cantera for the criteria set forth by the developers of the CRM code.

One difference between the CHEMKIN-II and CHEMKIN-III is the user interface. CHEMKIN-II does not have a GUI since originally it was intended for researchers and scientists (although it can be compiled on PC's), whereas CHEMKIN-III is a commercial

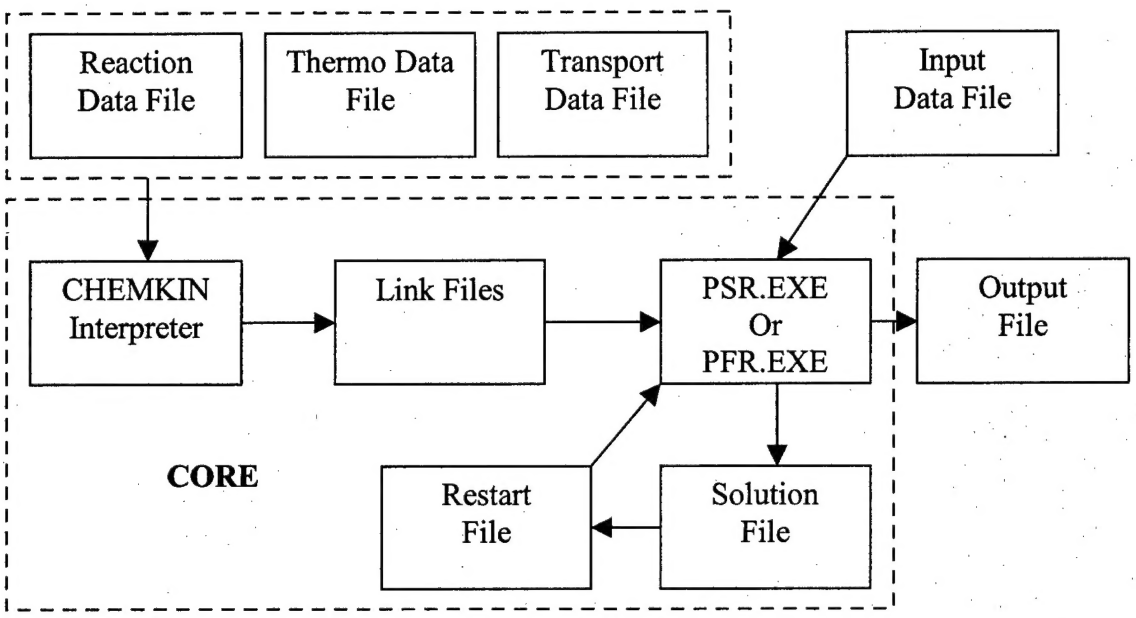

Figure 1. Module Interaction for CHEMKIN, MODLINK and Cantera Codes.

	CHEMKIN II	CHEMKIN III	MODLINK	CANTERA
Cost of Software	None	Fee	Fee	None
User Interface	Command Line	GUI	GUI	Command Line
Technical Support	None	Yes	Yes	Limited
Demonstration Software	Software is Free	Yes	Yes	Software is Free
Code Validation	Yes	Yes	Yes	Limited
Post Processing	User Specified	Built-in	Built-in	User Specified
User Subroutines	Yes	Not without Permission	Not without Permission	Yes, Limited

Table 1. Summary of CRM Survey

package, and its interface and platform is more user-friendly. This maybe an advantage to the casual user, but for an engineer looking to model a gas turbine engine, CHEMKIN-III, (as a package) does not allow user subroutines without permission from Reaction Design. The previous statements also holds true for MODLINK, when compared with CHEMKIN-II. Due to its ability to link with user subroutines, availability, and user interface, CHEMKIN-II is chosen from the three codes discussed above.

Cantera is an open source software package capable of solving chemically reacting flow for stirred tank reactors currently in development by Professor David Goodwin at California Institute of Technology. Cantera is available for use in many programming languages and interfaces, such as FORTRAN, C++, MATLAB, and Python, which may aid in the development of additional code that will be needed to implement the CRM

scheme. Although Cantera was originally developed for the chemical process industry, it is gaining support in the combustion community. Unfortunately, currently there is no PFR code available for Cantera, which therefore makes it unsuitable for the development of the CRM at this juncture.

The authors chose CHEMKIN II to be the source code for the CRM. CHEMKIN II was chosen because of its availability (open source code), ability to add subroutines (liquid spray model, soot production), and the available validation data. The only drawback of CHEMKIN-II, its lack of a GUI, actually makes it easier to recompile the code, and makes it easier to add subroutines. Hence, the use of CHEMKIN-II for the developmental stage of the project will aid in speeding up the process.

Task 2: Integrate PSR and PFR reactor codes, and construct reactor networking pathways.

In order to complete this task, the researchers developed a software driver program that allows the user to mix and match combinations of PSRs, PFRs, and mixing regions to simulate a GTE combustor. The researchers have developed:

- List of input file parameters to fully describe the network of reactors
- FORTRAN (Specification) subroutine to read and create input data
- FORTRAN (Parser) subroutine to link PSR and PFR modules

Figure 2 shows the overall program structure for the software. The specification file reads the inlet and reactor parameters. Any calculations necessary to transform the inlet and reactor parameters, such as unit changes or non-dimensionalization of values, are also performed. Based on these parameters, an input file is created for the core software chosen in Task 1. The core software consists of the PSR and PFR subroutines, which in turn use CHEMKIN–II to perform the kinetics calculations. The output from the core software is parsed in a subroutine to determine further actions, and is a foundation for optimization subroutines (for optional Task 6).

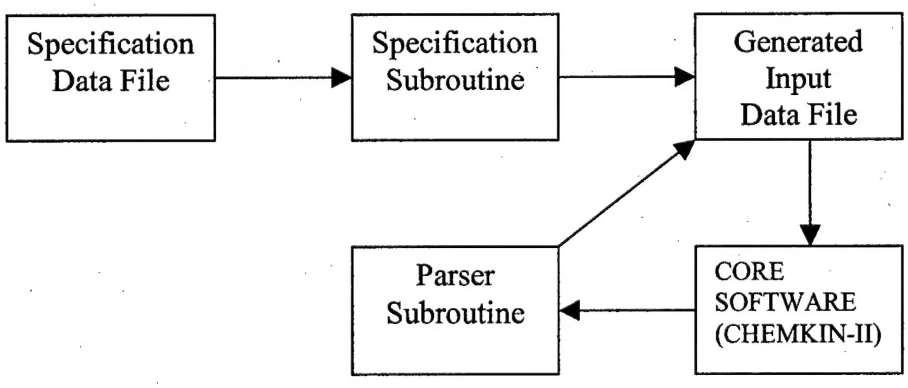

Figure 2. CRM software driver program.

This software allows for the combination of PSRs, PFRs, and mixing zones in any combination or sequence. The user specifications in this initial data file include:

- Inlet conditions (temperature and pressure) for the main air and fuel
- Inlet conditions (temperature and pressure) for the cooling air (such as for the dome or liner)
- Initial equivalence ratio
- Residence times of the various reactors.

The user specifications become more complicated as the number of inlet flows into the combustor increases.

The Parser subroutine calculates the flow parameters for the user designed CRM network. This subroutine must account for the separation and recombination of flows (through various inlets to the combustor or in different regions of the combustor) to generate the required input condition to the CRM submodule.

In many regions of the combustor, flows of differing composition and properties (mass flow rate, temperature, pressure, etc) are mixing. The parser subroutine and a mixing module have been developed to compute the properties of the resultant mixture. The composition of the mixture is computed and normalized into mass or mole fractions to be used as input into the CRM models. The mixture temperature is obtained from an energy balance, using an iterative procedure to extract the mixture temperature.

Task 3: Demonstrate the CRM network code's ability to predict data that exists for lean-premixed combustors.

A lean, premixed can combustor (known as Combustor A) that was studied extensively by researchers for the Department of Energy's Advanced Gas Turbine System Research Program [7, 8] was used as the first validation case. A schematic of this combustor showing the CFD calculated flow field is given in Fig. 3. This combustor is operated at approximately 10 atmospheres with an inlet air temperature of 645 K (702°F). Pre-mixed fuel (methane) and air enter the head-end through a swirler, and dome and liner cooling flows enter at multiple wall locations. The CFD case with a pilot shown is not the case modeled here, which had no pilot. The test conditions modeled and corresponding experimental measurements are listed in Table II.

The CRM network that was used to model combustor A is shown in Fig. 4. The primary reaction zone is modeled as two PSR's: PSR 1 reacts a small percentage of the fuel at a fixed equivalence ratio of 0.8 to simulate the effect of unmixedness, in which fuel-rich pockets can persist and combust (combustor A operates with substantial unmixedness [9, 10], and PSR 2 reacts the balance of the fuel and head-end primary air. The percentage of fuel split to PSR 1 is varied with condition in a linear fashion (corresponding to main zone equivalence ratio (φ))) to reflect a similar variation in the measured combustor A unmixedness [9]. A portion of the PSR 2 output is mixed with the dome cooling air and reacted in PSR 3. The output from all three PSR's is then mixed and split between "core" and "wall" flow paths. The "core" path is modeled as a PFR with no additional inputs,

while the "wall" path is modeled as two PFR's in series with wall cooling air added to each. The output from these flow paths is then mixed and added to a "quench" PFR. Finally "quench" or dilution air is mixed in and the final concentrations and temperature are calculated.

TABLE II. Combustor A Test Conditions and Measured Pollutant Concentrations

Case	Overall φ	Air Flow	Fuel Flow	T air	T fuel	P	NOx	CO
		(kg/s)	(kg/hr)	(K)	(K)	(atm)	ppm @ 15% O2	ppm @ 15% O2
1	0.41	1.19	106.9	649	294	9.8	101.51	1.42
2	0.37	1.20	97.38	646	294	9.9	76.79	0.72
3	0.32	1.19	83.26	645	295	10.0	56.11	0.43
4	0.28	1.19	72.53	645	296	9.9	33.16	4.43
5	0.25	1.17	63.85	646	299	9.9	20.95	125.47
6	0.23	1.19	59.18	646	299	9.9	12.3	896.08

Initial values for the various model parameters are based on CFD results for one test condition and then tuned for best match between model output and the experimental data. Best values for those parameters that are held constant from case to case are listed in Table III. PSR residence times and PSR1/PSR2 fuel split are varied from case to case, and are listed in Table IV. Initial estimates of PSR residence times (τ) were based on minimum time for blowout. The residence time in PSR3 is considerable longer than for PSR1 and PSR2 because the PSR3 temperature is much lower due to the addition of the dome cooling air (PSR3 is also a small contributor to NOx and CO emissions).

Table III. Model Constant Parameter Values

Parameter	PFR 1 τ	PFR 2 τ	PFR 3 τ	PFR 4 τ	Split 1	Split 2
Value	1.5e-2 sec	1.0e-2 sec	5.0e-3 sec	5.0e-3 sec	0.75	0.5

Table IV. Model Variable Parameter Values

Case	PSR 1 Fuel Split	PSR 1 τ	PSR 2 τ	PSR 3 τ
		(sec)	(sec)	(sec)
1	0.199998	2.0e-5	2.0e-5	1.05e-2
2	0.169353	2.5e-5	2.5e-5	1.05e-2
3	0.132579	4.5e-5	4.5e-5	1.05e-2
4	0.077418	1.1e-4	1.1e-4	1.05e-2
5	0.034515	3.0e-4	3.0e-4	1.05e-2
6	0.009999	6.1e-4	6.1e-4	1.05e-2

The resulting model predictions of NOx and CO emissions are compared to the measurements in Figures 4and 5 below. The CRM network captures both the trends and values of the emissions quite accurately over a wide range of equivalence ratios.

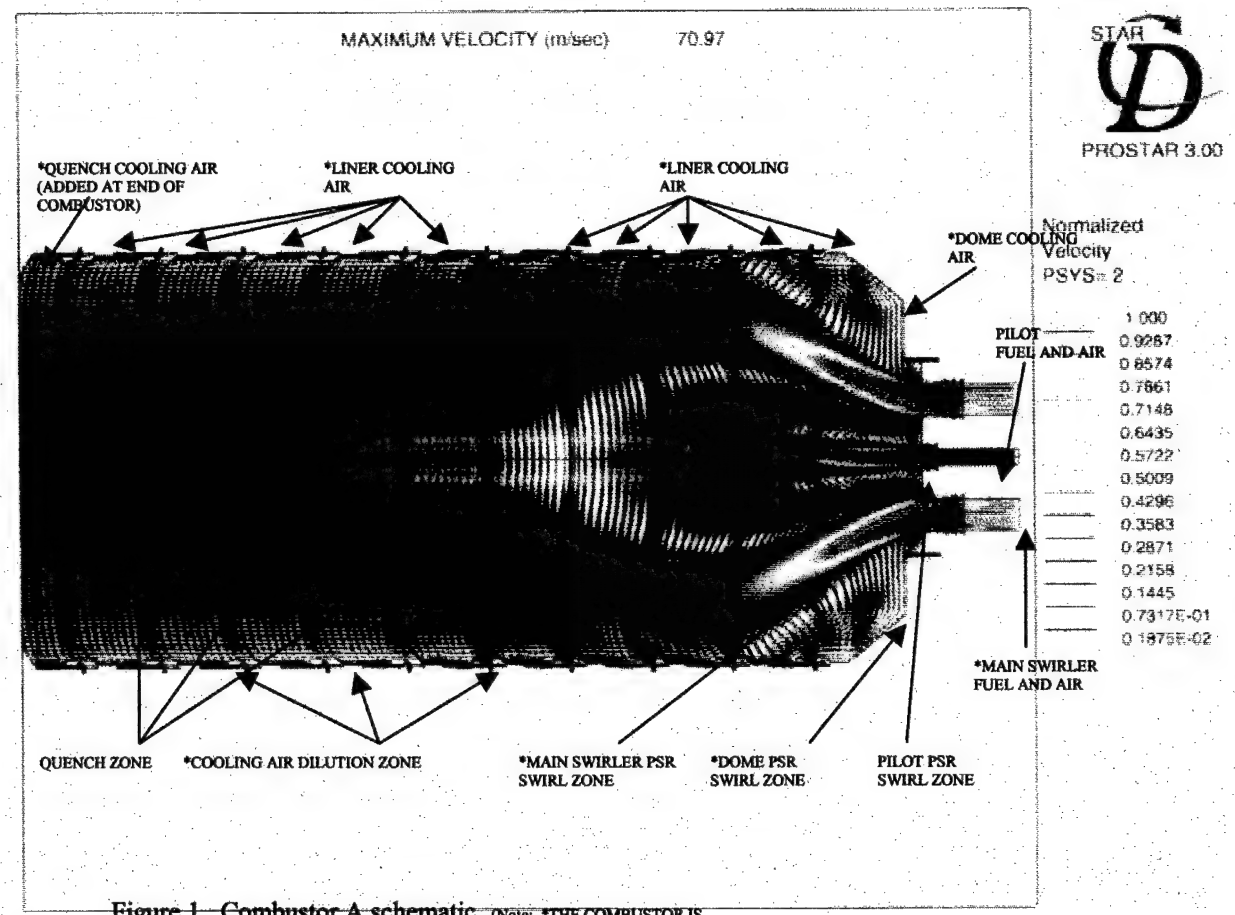

Figure 1. Combustor A schematic. (Note: *THE COMBUSTOR IS AXIALLY SYMMETRIC)

Figure 1 ~~AXIALLY SYMMETRIC~~) profile for test point 1.

Figure 3. CFD predictions of flowfield in Combustor A.

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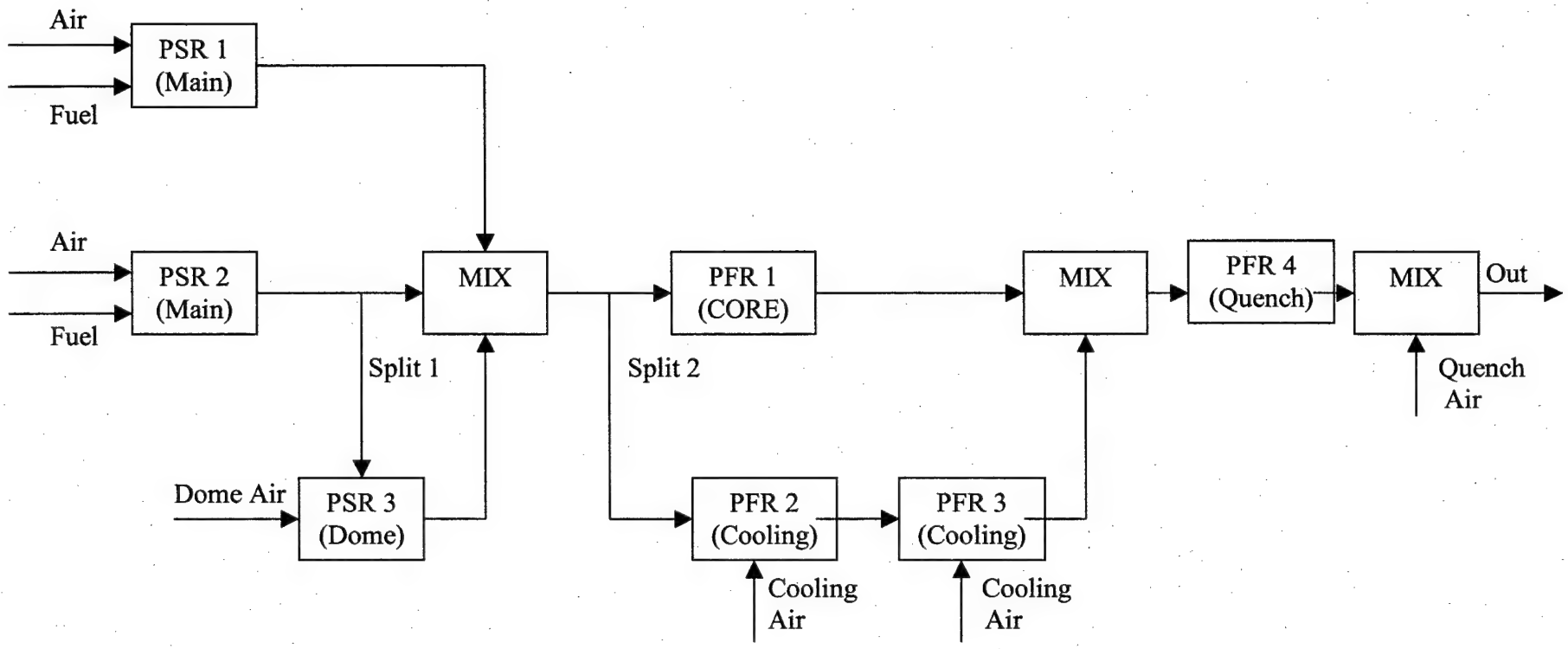


Figure 4. CRM Network of Combustor A. The main combustion zone is split into two PSRs to account for imperfect premixing.

Figure 4. Comparisons of CRM network NOx predictions to experimental measurements.

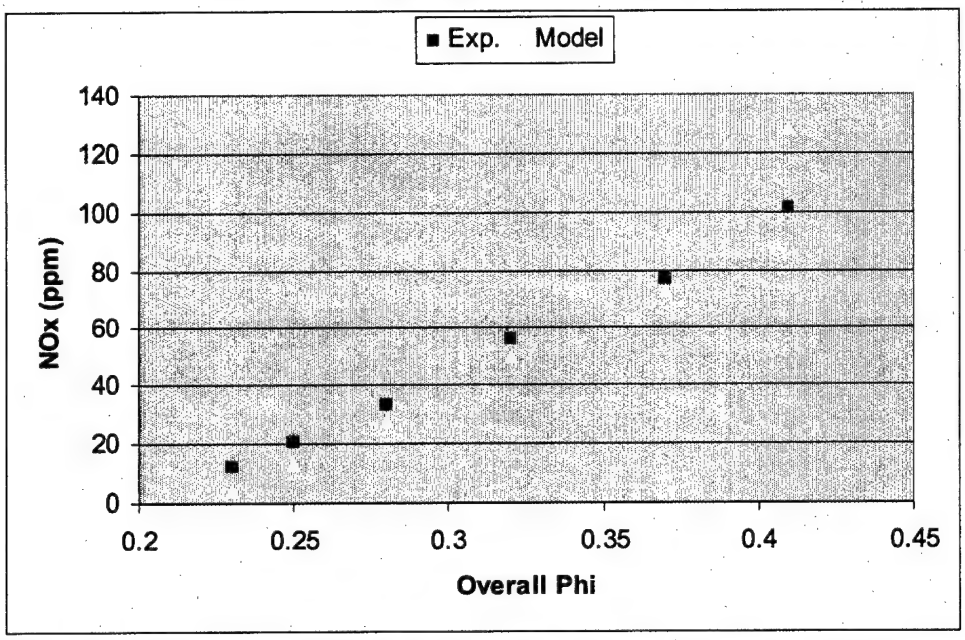
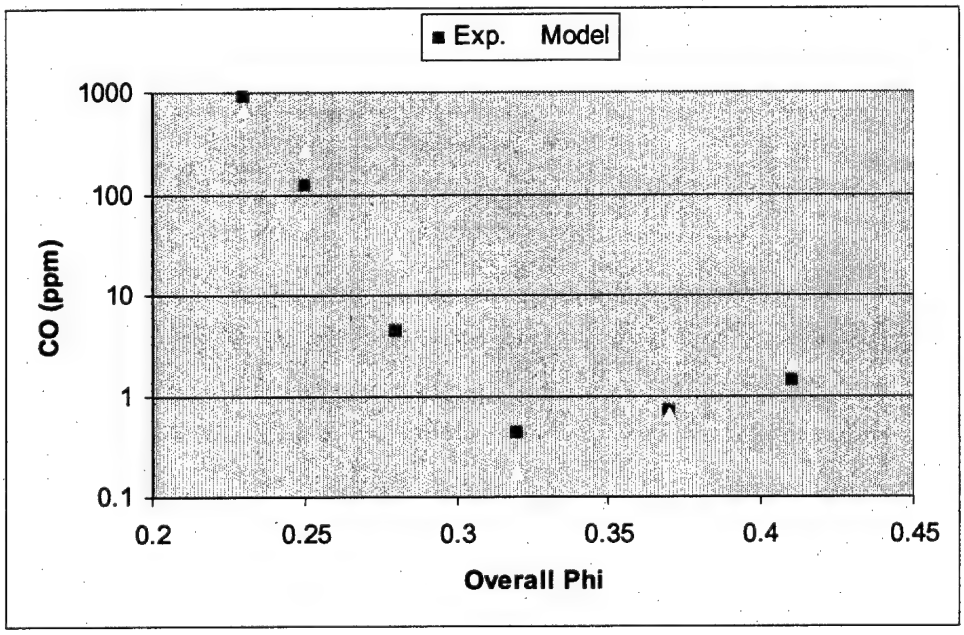


Figure 5. Comparisons of CRM network CO predictions to experimental measurements.



Task 4: Demonstrate the ability of the CRM network code to predict the non-linear response of combustor parameters to change in FAR, and identify parameters that have most affect on the performance of a high FAR combustor.

A CRM network model was developed to model a standard aero-combustor for which data was available. The combustor input parameters and experimental measurements are summarized in Tables V and VI. The network is shown in Figure 6 overlaid on a schematic of the combustor to show the relationship between the various reactors and combustor zones. The primary reaction zone (from the head-end to the primary jets) is modeled as a pair of PSR's to simulate spray combustion and uses all of the dome, dome cooling, and primary jet air. The first PSR models diffusion limited combustion taking place around droplets of fuel, and is operated at an equivalence ratio of 1.1, while the second PSR models well-mixed combustion resulting from complete droplet vaporization prior to burning. The fuel split between the two PSR's is an adjustable parameter. The first PSR uses as much air as necessary for combustion at the specified equivalence ratio of 1.1, with the remainder of the dome air, the dome cooling air, and primary jet air added to the second PSR. Note that as the engine operating point changes, the fuel split may vary to take into account changes in spray characteristics. The zone downstream of the primary jets is modeled as two PFR's in parallel, one for the core flow, to which the wall cooling air does not penetrate, and one for the near-wall flow, which is diluted by wall cooling air and the quench air. A final PSR recombines these two flows prior to exiting the combustor. This modeling used a chemical kinetic mechanism for n-heptane (as a surrogate for JP8) based on that of Warnatz [11] to which the NOx chemistry from GRImech3.0 was added.

Table V. Aero Combustor Operating Points and Measured Emissions

Case	Air Flow	Fuel Flow	Overall FAR	T in	P in	NOx	CO
	(lbs/sec)	(lbs/hr)		(°F)	(psia)	(EI)	(EI)
100% power	4949.5	51.9	0.0265	879	302.7	30.1	0.17
30% power	1436.7	26.7	0.0149	584	143.8	8.8	1.5

Table VI. Aero Combustor Air Flow Splits

Flow Splits	Dome	Dome Cooling	Primary Jets	Wall Cooling	Dilution
Specified (%)	11.5	8.8	13.8	30.1	35.8
CRM Network (%)	PSR1, excess to PSR 2	PSR2	PSR2	12% to PSR2, 88% to wall PFR	Wall PFR

Data was also available for a case in which the aero-combustor was modified by changing the air flow splits to direct more air into the head-end. Model cases were run for this modified geometry as well, and the flow splits are summarized in Table VII.

Figure 6. Aero Combustor and CRM Network

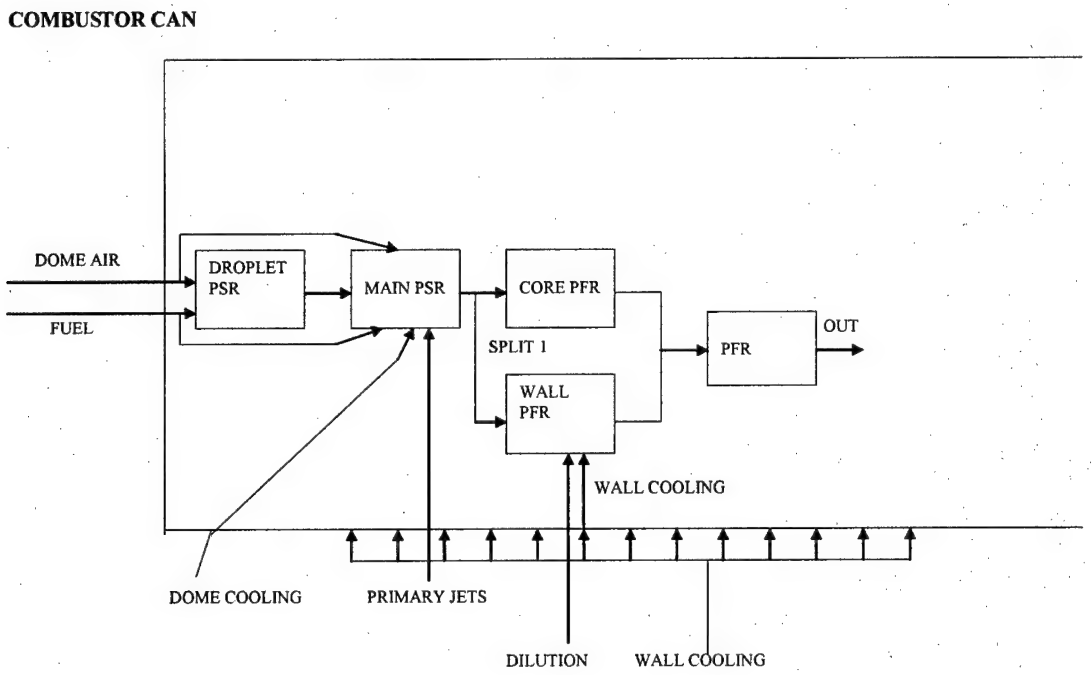


Table VII. Modified Aero Combustor Air Flow Splits

Flow Splits	Dome	Dome Cooling	Primary Jets	Wall Cooling	Dilution
Specified (%)	46.8	8.8	13.8	30.1	0
CRM Network (%)	PSR1, excess to PSR 2	PSR2	PSR2	12% to PSR2, 88% to wall PFR	Wall PFR

Residence times and network flow splits (fuel split and core/wall split) are adjustable parameters in this model with geometry and PSR blowout times used as guidance for initial guesses. The values used in the results presented below are listed in Table VIII.

Table VIII. Model Parameters

Case	Fuel split	PSR 1 τ	PSR 2 τ	Split 1	PFR 1 τ	PFR 2 τ	PFR 3 τ
	(% to PSR1)	(sec)	(sec)	(% to core)	(sec)	(sec)	(sec)
100% power	25	4e-4	9e-4	15	2e-2	2e-2	1e-3
30% power	25	4e-4	9e-4	15	2e-2	2e-2	1e-3

The results of the CRM network modeling are listed below in Table IX for both the aero combustor and the modified aero combustor described above. The model predicts the NOx emissions very accurately, and also tracks the CO emissions quite well (it over predicts for the 30% case, although it captures the trend correctly). The trends observed are the following:

- NOx emissions fall as power is decreased, which is due to the lower FAR (and thus reduced primary combustion zone temperatures) at reduced power.
- NOx emissions fall as increased air to the head-end leans out the combustion in the modified case, although the effect is not as great in the 30% case compared to the 100% case since the FAR is already considerably lower. This is illustrated in Figure 2 for the 100% case, which shows the effect of shifting dilution air to the head end. The 100% operating points for both the modified and unmodified cases are indicated, and bracket a maximum in NOx emissions. This maximum occurs as the equivalence ratio in the main combustion zone (PSR2) approaches 0.9 (Figure 3).
- CO emissions increase as power is decreased, due to primary combustion zone conditions closer to blowout and reduced CO burnout at the lower temperatures associated with the lower FAR.
- CO emissions increase drastically for the modified case at 30% power as the FAR in the head-end becomes still lower. At 100% power CO emissions are low in both cases as the primary zone is not close to blowout and not much CO is produced. Figures 7 and 8 show that CO emissions are not very sensitive to air distribution over the range of distributions covered by the 100% modified and unmodified cases.

It should be emphasized that not only does the CRM network model capture these trends, it also aids in their understanding as CO and NOx production at various points in the network can be examined. This is shown in Figures 9 and 10, in which it can be seen that conditions in the main combustion zone (PSR2) are critical in determining NOx emissions. One can also see that CO burnout does not occur in the 30% power case.

Table IX. CRM Network Modeling Results Compared to Experimental Measurements for the Standard Aero Combustor and the Modified Standard Aero Combustor

Case	Model NOx (EI)	Model CO (EI)	Meas. NOx (EI)	Meas. CO (EI)
Aero Comb. 100%	29.4	0.126	30.1	0.17
Aero Comb. 30%	7.0	9.94	8.8	1.5
Mod. Aero Comb. 100%	15.37	0.09	15.3	0.13
Mod. Aero Comb. 30%	6.48	128	7.0	12.9

Equilibrium calculations were also carried out for the aero combustor cases:

- NOx fell from 2,100 ppm to 1.5 ppm for the 100% and 30% power cases, a decline several orders of magnitude greater than observed.
- CO fell from 138 ppm to sub ppb levels for the same cases, a decline opposite to the trend observed.

Clearly NOx and CO emissions are not the results of equilibrium, and equilibrium calculations cannot correctly predict the emission trends of these pollutants.

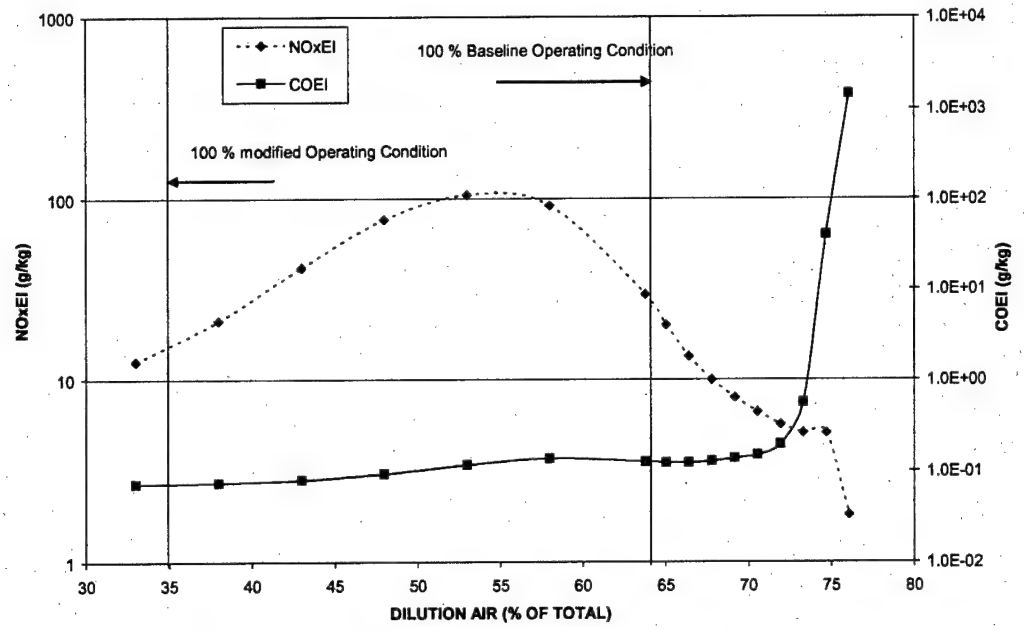


Figure 7. Effect of dilution on NOx and CO emissions. Operating points for the aero combustor 100% power and modified aero combustor 100% power conditions are indicated.

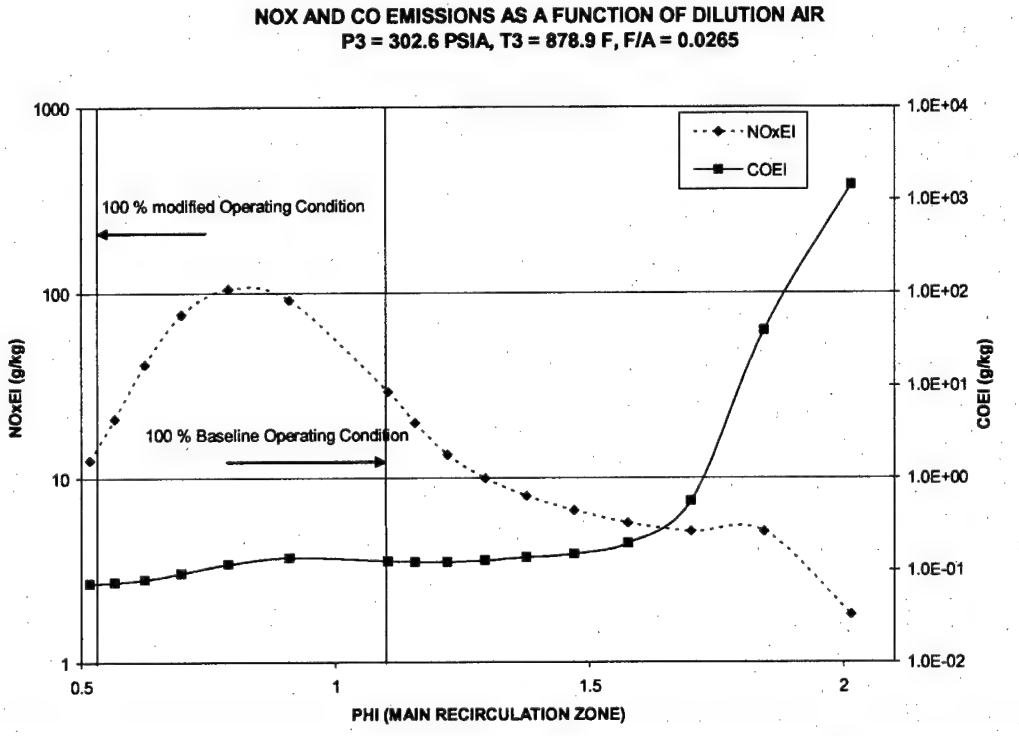


Figure 8. Main combustion zone (PSR2) equivalence ratio as dilution is varied (same data as Fig. 2) for the aero combustor 100% power and modified aero combustor 100% power conditions (indicated).

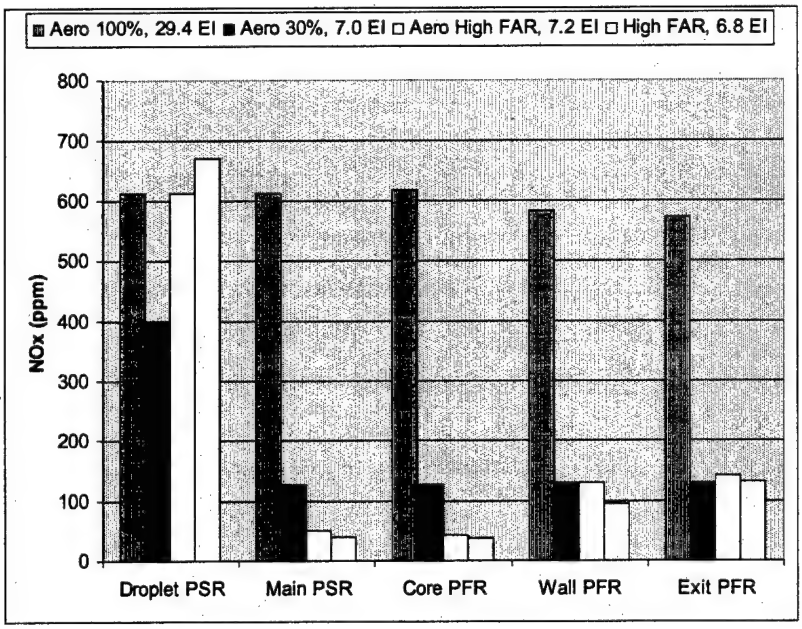


Figure 9. NOx concentration in the various network reactors for the aero combustor at 100% and 30% power, the aero combustor operated at standard conditions with high FAR, and the aero combustor operated at "high FAR" conditions (Table VI).

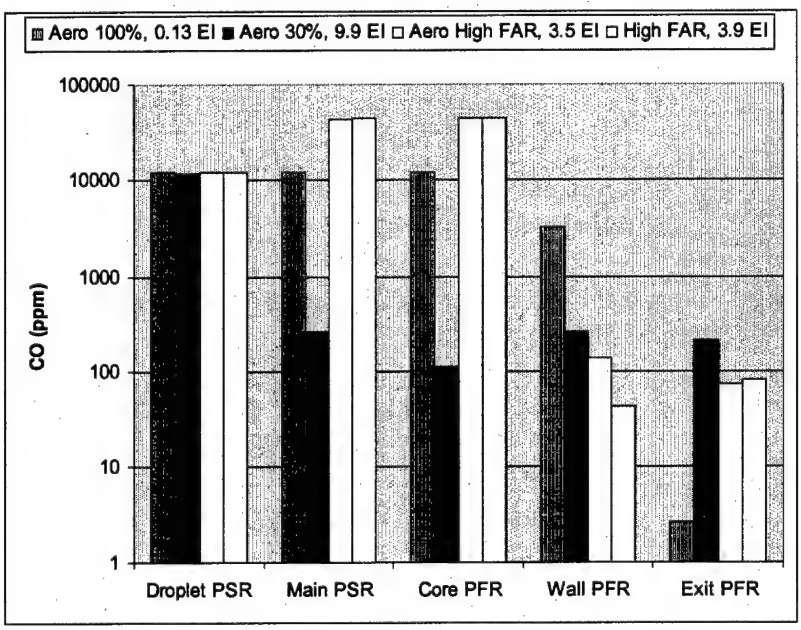


Figure 10. CO concentration in the various network reactors for the aero combustor at 100% and 30% power, the aero combustor operated at standard conditions with high FAR, and the aero combustor operated at "high FAR" conditions (Table VI).

High FAR and Geometry Effects

The CRM network described above was used to model high FAR combustion and to investigate the effects of geometry. The following cases were considered:

1. Base Case: Conventional combustor at 100% power (previous section)
2. Conventional combustor at High FAR
3. Modified combustor at High FAR
4. High FAR combustor (conventional geometry at high FAR conditions below)
5. Modified High FAR combustor (modified geometry at high FAR conditions below)

The high FAR operating conditions are summarized in Table X.

Table X. High FAR Operating Conditions

Case	Air Flow	Fuel Flow	Overall FAR	T in	P in
	(lbs/sec)	(lbs/hr)		(°F)	(psia)
100% power	54144	376	0.040	1001	588

The results of the CRM network modeling for these cases are presented below in Table XI. It can be seen that operating the standard combustor at high FAR (cases 2 & 5) actually reduces NOx emissions while increasing CO emissions. This is due to the fact that in the high FAR cases the primary zone (head-end) of the combustor is operated in a fuel rich condition. As shown in Figure 8, at equivalence ratios greater than 1 temperature and hence NOx emissions decrease, while CO emissions increase due to incomplete combustion. Increasing air to the head-end can then increase NOx emissions if the resulting primary zone equivalence ratio is brought closer to 1 (cases 3 & 5), which is the case for these conditions, as shown in Figures 11 and 12. These figures show that for the baseline high FAR condition, the main combustion zone is very rich. In the modified case, decreasing dilution air and adding it to the head-end results in near stoichiometric conditions in the main combustion zone. This results in high temperatures and high NOx production. CO emissions are not strongly affected by this change.

Table XI. FAR and Geometry Effects

Case	Model NOx	Model CO
	(EI)	(EI)
1) Aero Comb. 100%	29.4	0.126
2) Aero Comb. High FAR	7.24	3.52
3) Mod. Aero Comb. High FAR	97.5	3.36
4) High FAR Comb.	6.77	3.94
5) Mod. High FAR comb.	115.42	3.73

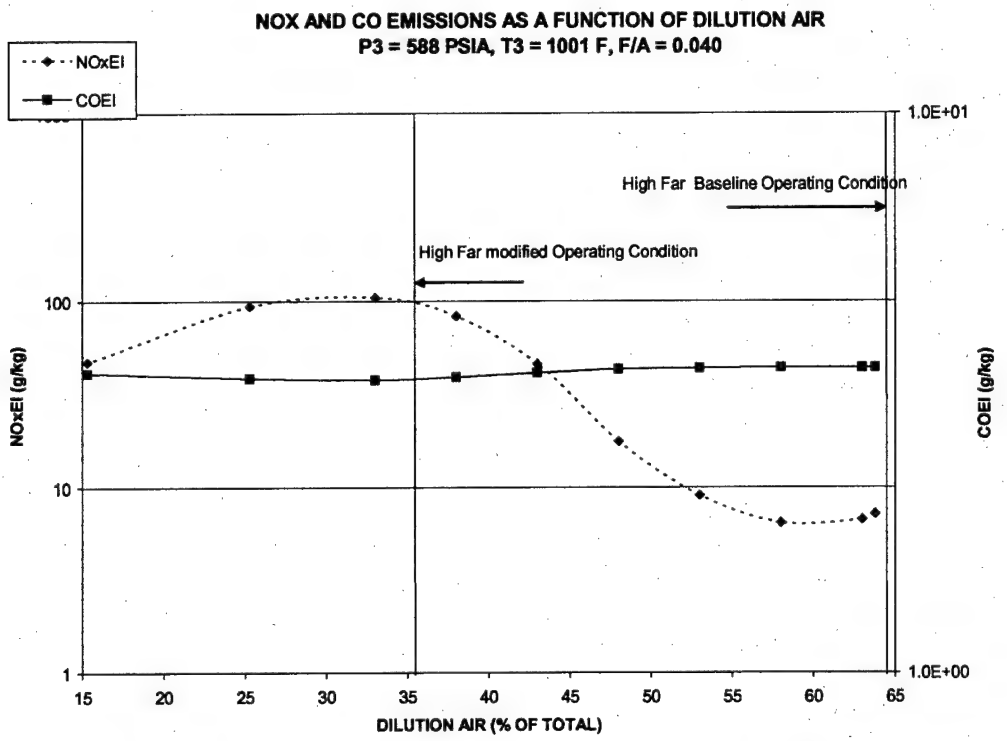


Figure 11. Effect of dilution on NOx and CO emissions. Operating points for the High FAR and Modified High FAR combustors are indicated.

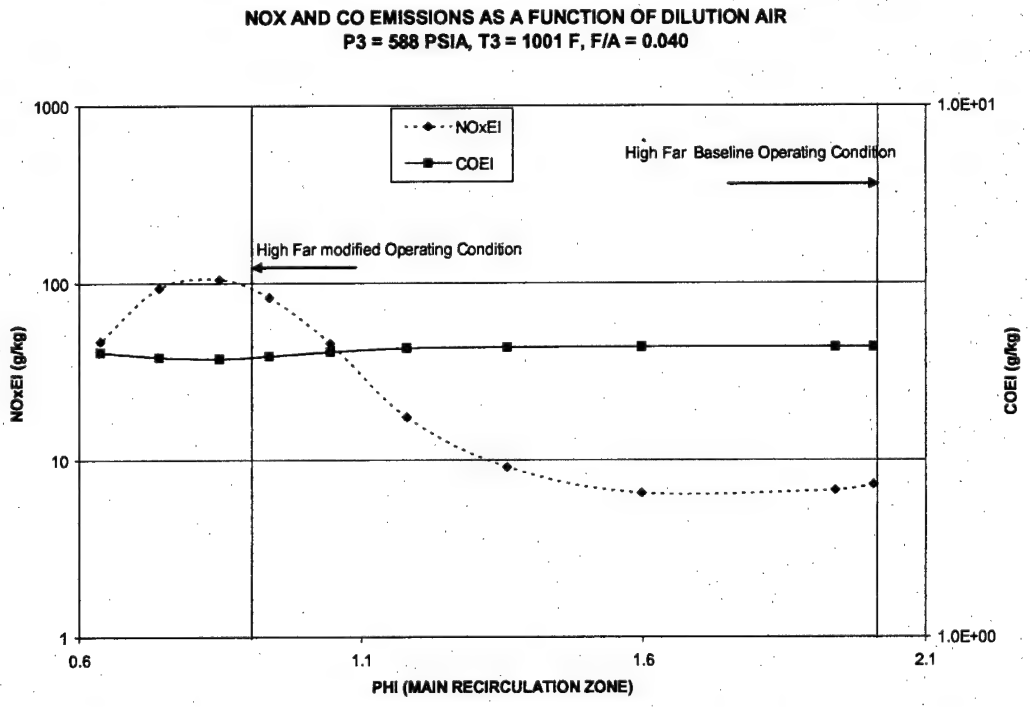


Figure 12. Main combustion zone (PSR2) equivalence ratio as dilution is varied (same data as Fig. 2) for the High FAR and Modified High FAR combustors (operating points indicated).

Figures 9 and 10 also show that at high FAR conditions, the lower temperature in the main combustion zone results in less NOx production at that location. This carries through to less NOx emitted, although some NOx is produced in the downstream region. CO is production in the main PSR is greatly increased, and although burnout occurs, CO emissions are higher. In the high FAR case, it is apparent that significant reaction is still occurring in the final PFR. The effects of geometry are shown in Figures 13 and 14. Transferring diluent air to the head-end results in operation of the main PSR at close to stoichiometric (Fig. 12), with resultant high temperatures and elevated NOx production. Although CO levels are reduced in the main PSR, significant CO carries through the PFRs.

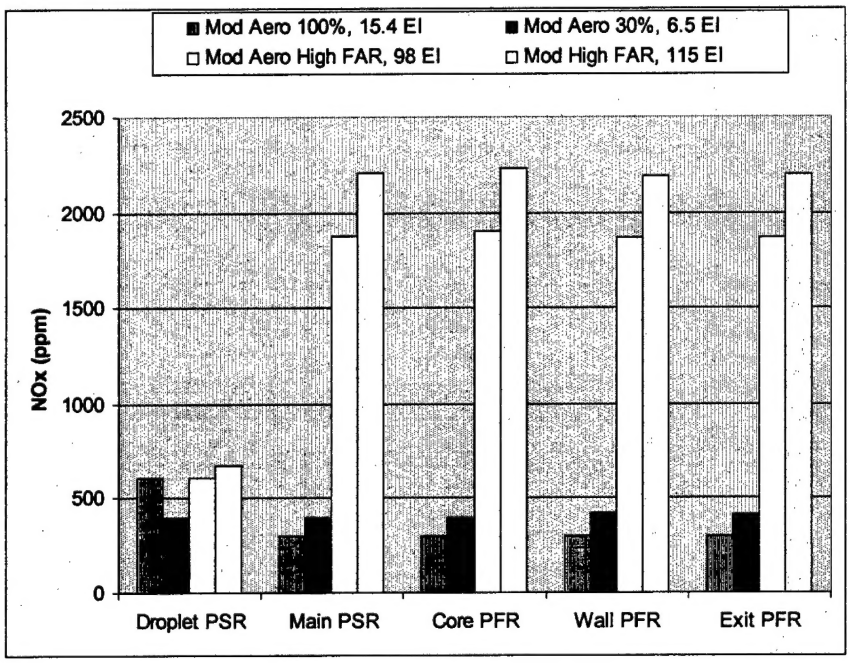


Figure 13. NOx concentration in the various network reactors for the modified aero combustor at 100% and 30% power, the modified aero combustor operated at standard conditions with high FAR, and the modified aero combustor operated at "high FAR" conditions (Table XI).

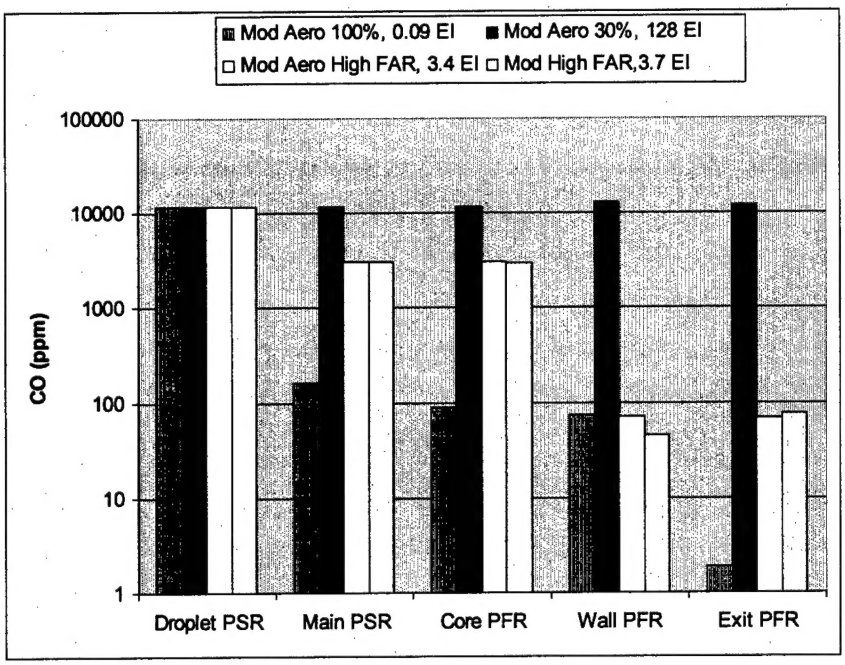


Figure 14. CO concentration in the various network reactors for the modified aero combustor at 100% and 30% power, the modified aero combustor operated at standard conditions with high FAR, and the modified aero combustor operated at "high FAR" conditions (Table XI).

Conclusions and Recommendations

A need exists for advanced kinetics-based modeling tools to assist engine builders in the design and development of high FAR engines. Combustion Science & Engineering, Inc. (CSE) has successfully demonstrated the feasibility of a flexible computational tool based on chemical reactor modeling (CRM) for the initial stages of gas turbine combustor design. Subroutines have been written in order to integrate PSR and PFR reactor codes, and to construct pathways for reactor networking. The code has been validated against experimental data for a conventional aircraft gas turbine combustor as well as a stationary gas turbine. The predictions of pollutant emissions show excellent agreement with the measurements, capturing both the magnitude and trends of the data. The input conditions to the CRM model of the aircraft combustor were extended to those of a High FAR combustor, with the expected increases in pollutant emissions and core combustion temperatures.

The results from the Phase I research have demonstrated a number of important features of CRM modeling and the potential benefits of this code to combustor designers.

- CRM modeling permits the designer to quickly study the effect of changing important inlet parameters, such as airflow splits, primary jet location etc., on combustor performance. The computational time of these calculations is order of magnitudes faster than comparable CFD studies. For example, CRM

computational time is on the order of minutes, while a reacting flow CFD model may take several days to converge.

- CRM modeling allows the use of full chemical kinetic mechanisms. This is especially important in High FAR combustors, where a wide range of fuel-air mixtures can be encountered in a given combustor. The important chemical reactions for flame ignition or pollutant formation are very dependent on the local proportions of fuel and air. This dependency is very difficult to capture using a reduced chemical kinetic mechanism, as reduced mechanisms are accurate for narrow range of conditions (e.g. pressure, temperature, fuel-air ratio). CSE is a leader in the development and implementation of reduced mechanisms in CFD codes, and is well aware of the conditions over which these mechanisms will provide accurate results. Proper implementation of a CFD based technique during the early stages of combustor design under High FAR conditions would be very time consuming, expensive and have limited accuracy.
- CRM modeling has applications across the entire range of gas turbines, including microturbines, stationary power generation turbines, and aircraft gas turbines.

CSE recommends the continued development of this design tool in a Phase II study. The Phase I results have shown great promise that a code can be developed which will assist design engineers develop more efficient combustors, while lessening the amount of testing and design time. CSE has received several letters of support from industry, recommending continued development.

During Phase II development, a number of issues must be investigated to improve the code and aid in making a user-friendly design tool.

- Additional Physical Phenomena Submodels
  - Liquid Fuel Droplet Vaporization to simulate spray combustion
  - Distribution of Equivalence Ratios to simulate variation in unmixedness.
  - Coupling Design Parameters to CRM variables
  - Soot/Smoke Production
- Development of a Graphical User Interface (GUI)
- Improvement of the Numerical Solvers

Further methodology development and validation is also necessary. Current discussions with aircraft gas turbine manufacturers, including those involved in the development of the Joint Strike Fighter, have indicated that these companies are willing to work with CSE to refine the CRM code. This cooperation will include access to experimental and analytical data against which CRM predictions can be compared. Furthermore, this interaction will be invaluable towards developing a methodology and interface that is most useful to the combustor design engineer.

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